

Interface-mediated pairing in field effect devices

V. Körting¹, Qingshan Yuan^{1,2,3}, P. J. Hirschfeld^{1,4}, T. Kopp¹, and J. Mannhart¹

¹Center for Electronic Correlations and Magnetism, EP6, Univ. Augsburg, Augsburg Germany

²Texas Center for Superconductivity and Advanced Materials, Univ. of Houston, Houston, TX 77204 USA

³Pohl Institute of Solid State Physics, Tongji University, Shanghai 200092, P.R. China

⁴Department of Physics, University of Florida, PO Box 118440, Gainesville FL 32611 USA

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We consider the pairing induced in a strictly 2D electron gas (2DEG) by a proximate insulating film with polarizable localized excitations. Within a model of interacting 2D electrons and localized two-level systems, we calculate the critical temperature T_c as a function of applied voltage and for different materials properties. Assuming that a sufficient carrier density can be induced in a field-gated device, we argue that superconductivity may be observable in such systems. T_c is found to be a nonmonotonic function of both electric field and the excitation energy of the two-level systems.

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Shortly after the publication of the BCS theory of superconductivity, W. A. Little proposed a possible pairing mechanism for electrons in long organic molecules involving localized electronic excitations in the molecules' side chains [1]. The suggested advantages of such an arrangement included the large characteristic energy of the couplings, which might lead to high temperature superconductivity (HTSC), and the separation of the excitations themselves from the screening effects of the electron gas. Such a pair mechanism has never been realized, presumably due to large fluctuation effects in quasi-1D systems. Later, Ginzburg [2] and Allender, Bray and Bardeen [3] proposed a similar excitonic 2D mechanism in superconductor-semiconductor sandwiches. The enormous body of early work on this problem has been reviewed in [4]. One problem with these schemes is clearly that the localized nature of the excitations implies that at most one or two atomic layers of the intercalating insulator can contribute to the pairing, meaning that the enhancement of pairing in the relatively thick nearby superconductor is negligible.

Here we propose that a similar scheme might work for an insulating layer in proximity with a superconducting layer of near-atomic thickness. Such systems can in principle be prepared in several ways, but the most promising is perhaps the field effect method pioneered in the early 90's with the intent of increasing the carrier density and hence T_c in HTSC cuprate devices [5, 6, 7, 8, 9]. This work has shown incontrovertibly that T_c and other superconducting properties in metallic samples can be influenced by an applied gate voltage. While the experiments have most often been interpreted in terms of electronic structure variations near the interface, they are not understood in detail.

It is interesting to ask if new physics can result from field doping of insulators. In the most recent reports on field-doping of SrTiO₃, Pallecchi *et al.* [10] and Ueno *et al.* [11] were able to achieve an areal carrier density of ~ 0.01 – 0.05 per unit cell. It is difficult to achieve higher densities due to electrical breakdown in the insulating layer at high fields. But there seems to be no *fundamen-*

tal objection to even higher charge densities, since complex oxide dielectrics and ferroelectric oxides can achieve polarizations in the range of ~ 0.5 [8]. In fact, very recently the first observation of field-induced superconductivity was reported for a device with a Nd_{1.2}Ba_{1.8}Cu₃O₇ epitaxial film grown on SrTiO₃ substrates [12].

Therefore one may legitimately ask the question what critical temperature can be achieved in a system where the pairing comes entirely from the excitations in the proximate insulating layer, and how T_c is likely to vary with field in this case. Alternatively, one can assume the existence of a 2D superconducting layer with pre-existing pair interaction and bare critical temperature T_c^0 , and ask by how much the presence of the insulating layer enhances T_c . While in a strictly 2D system the T_c 's referred to cannot correspond to true long-range order, the creation of a field-tuned superconducting state with algebraic order at finite temperatures would be of considerable interest and applicability in small devices.

We begin by considering an insulating amorphous film $L1$ in proximity to a correlated insulator $L2$ (drain-source (DS) channel of a field effect device), similar to Ref. 12, with a small density of localized charge carriers. Applying an electric field as shown in Fig. 1 sweeps charge carriers to the interface with the film $L1$ where they accumulate [13]. The formation of the 2D band induced by an electric field has been studied by Poilblanc *et al.* [14]. We assume for the moment that in the absence of the film $L1$ there are no pairing interactions between the electrons in the material $L2$. Qualitatively, we expect the following picture to apply: virtual excitations in the dielectric $L1$ induce Cooper pairing in the adjacent layer $L2$. The critical temperature must increase initially with the field since carriers are being injected into the system. With increasing electric field the larger level splitting of the two level system leads to a suppression of the polarization fluctuations and the pair potential decreases. T_c is therefore expected to reach a maximum at a characteristic field strength; it is our objective to estimate the scale of possible T_c 's through this process, as well as the field strength required to attain it.

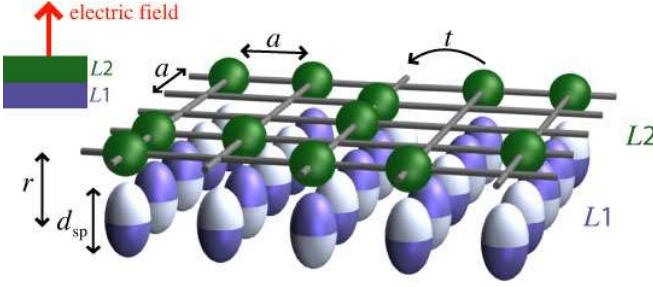


FIG. 1: Our model of a field effect transistor is represented by two layers (L1 and L2):

L1: dielectric layer with local dipoles of dipole moment ed_{sp} , presented by two-level systems;

L2: metallic DS-channel with a 2D electron gas.

We now propose a crude but concrete framework within which one can calculate these effects. Roughly speaking, the dielectric can have two effects on T_c . First, it can reduce the Coulomb pseudopotential of electrons in the field-doped layer due to the large dielectric constant of the amorphous insulator L1. We are more concerned here with the second effect, namely an additional contribution to the residual pairing interaction at the interface due to virtual polarization of the dielectric itself.

I. MODEL

The Hamiltonian we consider describes a single layer L2 of electrons c_i^\dagger hopping on a square lattice with lattice constant a , nearest neighbor hopping t , and a set of localized two-level systems in an adjacent layer L1 with ground state s_i^\dagger and excited state p_i^\dagger separated in energy by Δ_{sp} , and their respective dipole moment is ed_{sp} (Fig. 1). Note these states simply designate ground and excited states of a localized two level system, and need not correspond to actual atomic s- and p- orbitals. To ensure that the two-level system is occupied by only one electron, the constraint $s_i^\dagger s_i + p_i^\dagger p_i = 1$ must be enforced. The electric field

$$\mathcal{E} \equiv E_{sp}/(e d_{sp}) \quad (1)$$

is assumed to populate the metallic layer and simultaneously polarize the two level systems by driving transitions between the s and p states, which are coupled to the free electrons in the layer L2 by a contact interaction V_{sp} .

The Hamiltonian contains, according to our assumptions, the following elementary processes:

$$H_{tot} = H_t + H_{2l} + H_{ext} + H_{int} + H_\mu + H_{e-e} \quad (2)$$

with

$$H_t = -t \sum_{\langle ij \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} \quad (3)$$

$$H_{2l} = \frac{1}{2} \Delta_{sp} \sum_i (p_i^\dagger p_i - s_i^\dagger s_i) \quad (4)$$

$$H_{ext} = E_{sp} \sum_i (p_i^\dagger s_i + s_i^\dagger p_i) \quad (5)$$

$$H_{int} = V_{sp} \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} (p_i^\dagger s_i + s_i^\dagger p_i) \quad (6)$$

$$H_\mu = -\mu \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} \quad (7)$$

$$H_{e-e} = U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}. \quad (8)$$

Here H_t describes a band of noninteracting 2D electrons on a square lattice, H_{2l} the energies of the localized two level system, H_{ext} the coupling of the electric field to these orbitals, H_{int} the Coloumb interaction between electrons in the metallic layer and the two level system, and H_μ the chemical potential. The direct electron-electron interaction term H_{e-e} is taken to be local and repulsive. Very similar models have been used recently to discuss dielectric properties of bulk cuprates [15], the competition between charge density wave and superconductivity in two dimensional electronic systems [16], and superconductor-ferroelectric multilayers [17]. The system is not exactly soluble, but will be treated under the assumption that the polarization through the charges in L2 is not large enough to drive the system into the ferroelectric state. We first diagonalize $H_{2l} + H_{ext}$, and then express the corresponding quasiparticle operators in a pseudospin representation where S_i^z measures the occupation of the 2-level system and S_i^\pm induces transitions between the two eigenlevels. The occupation constraint on the two-level system is preserved by the usual spin algebra. The (exact) final form of the Hamiltonian is

$$H_{2l} + H_{ext} = -2\sqrt{E_{sp}^2 + (\frac{1}{2}\Delta_{sp})^2} \sum_i S_i^z \quad (9)$$

$$H_{int} = -V_z \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} S_i^z \quad (10)$$

$$+ V_x \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} (S_i^+ + S_i^-) \quad , \quad (11)$$

where

$$V_z = 2V_{sp} \frac{E_{sp}}{\sqrt{E_{sp}^2 + (\frac{1}{2}\Delta_{sp})^2}}$$

$$V_x = V_{sp} \frac{\frac{1}{2}\Delta_{sp}}{\sqrt{E_{sp}^2 + (\frac{1}{2}\Delta_{sp})^2}} \quad .$$

The system of interacting spins-1/2 and fermions may now be treated within linear spin wave theory, an ap-

proximation which is justified *a posteriori* by the observation that the occupation of the higher-energy 2-level state is very small, due to the sufficiently large 2-level splitting [18]. Introducing the usual Holstein-Primakoff bosons [19], we make the approximate replacements $S_j^+ \rightarrow b_j$, $S_j^- \rightarrow b_j^\dagger$, $S_j^z \rightarrow \frac{1}{2} - b_j^\dagger b_j$ to find

$$H = -t \sum_{\langle ij \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} - \mu_r \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} - E_{2l} \sum_i \left(\frac{1}{2} - b_i^\dagger b_i \right) + V_z \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} b_i^\dagger b_i + V_x \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} (b_i + b_i^\dagger) + H_{e-e} \quad (12)$$

We have introduced the energy splitting of the two-level system

$$E_{2l} = 2\sqrt{E_{sp}^2 + \left(\frac{1}{2}\Delta_{sp}\right)^2} \quad (13)$$

and the chemical potential has been renormalized $\mu_r = \mu + V_z/2$.

We now declare that the Hamiltonian H is as good a starting point as (3)–(8) provided $\langle b_j^\dagger b_j \rangle \ll 1$. We therefore proceed to apply a Feynman variational procedure to the exact H , Eq. (12), after a unitary transformation, and attempt to extract the pairing mechanism. The dominant term for this mechanism is the term with V_x which, as in the phonon-induced superconductivity, produces Cooper pairing in second order perturbation theory [1]. However, for the field strengths which we will consider, the term with V_z is also not negligible and it will alter pairing in one significant respect: since it modifies the 2-level splitting when a charge carrier occupies the site coupled to the considered 2-level system, it will either increase the pairing interaction (for reduced splitting, i. e., negative V_z) or decrease pairing (for enhanced splitting, i. e., positive V_z) — an observation which may be derived straightforwardly from a mean field decoupling. For the physical system that we consider, E_{sp} and V_{sp} always have the same sign, and consequently V_z is positive [20]. All of the above considerations can also be derived in terms of states where charges in $L1$ are localized in states of definite position with respect to the interface, as depicted schematically in Fig. 1. In this representation, the V_z interaction may be shown to correspond to the repulsion of the electron in layer $L2$ and the field-induced dipole in $L1$.

In order to incorporate this effect we will include below the thermal average $V_z \sum_{i,\sigma} \langle c_{i,\sigma}^\dagger c_{i,\sigma} \rangle b_i^\dagger b_i = V_z n \sum_i b_i^\dagger b_i$ explicitly in the energy of the two-level system before handling the bosonic degrees of freedom. This is achieved

by rewriting the fourth term of Eq. (12)

$$V_z \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} b_i^\dagger b_i = -NV_z n n_b + V_z n \sum_i b_i^\dagger b_i + V_z n_b \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} + V_z \sum_{i,\sigma} \left[c_{i,\sigma}^\dagger c_{i,\sigma} - n/2 \right] \left[b_i^\dagger b_i - n_b \right] \quad (14)$$

where $n_b = \langle b_i^\dagger b_i \rangle$ is the number of bosons (the relative number of inverted 2-level systems per site), $n = (1/N) \sum_{i,\sigma} \langle c_{i,\sigma}^\dagger c_{i,\sigma} \rangle$ is the charge carrier density in layer $L2$, and N is the number of sites in $L2$. The second term on the right hand side accounts for a density-dependent renormalization of the two-level splitting:

$$E_{2l}^* = E_{2l} + nV_z. \quad (15)$$

In a first step we apply a Lang-Firsov (LF) transformation of the Hamiltonian H in order to identify the pairing interaction, and in a second step we control the decoupling of the interaction terms through Feynman's variational principle which also fixes the parameters of the LF transformation.

The LF transformation of the Hamiltonian $\tilde{H} = U^\dagger H U$ is achieved by the following unitary operator U :

$$U = \exp[-S_1(\theta)] \exp[-S_2(\gamma)] \quad (16)$$

with

$$S_1(\theta) = -\frac{1}{2V_x} \theta \sum_i (b_i^\dagger - b_i) \quad (17)$$

$$S_2(\gamma) = \frac{V_x}{E_{2l}^*} \gamma \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} (b_i^\dagger - b_i) \quad (18)$$

The parameters θ and γ will be fixed through the variation of the free energy. The standard form of the LF transformation for the Holstein model takes $\theta = 0$ and $\gamma = 1$. With a “zero-phonon” approximation the (phononic) Holstein model accounts for exact results in the antiadiabatic limit $E_{2l}/t \gg 1$. The variation of the parameters θ and γ has been devised in order to reproduce the adiabatic limit of the Holstein model as well [21, 22, 23, 24]; the static case is realized with $\gamma \rightarrow 0$ and with a finite θ which signifies a displacement field. For the Holstein model, a second canonical transformation of Bogoliubov type $U_B = \exp[-\alpha \sum_i (b_i^\dagger b_i^\dagger + b_i b_i)]$ is sometimes applied to allow for the anharmonicity of the lattice fluctuations. For our model, we have to suppress states with two bosons (corresponding to our initial constraint for the 2-level system), and subsequent variation of the free energy shows that in fact $\alpha = 0$. Also the “static displacement” should be suppressed since we do not intend to consider a finite static polarization. We verified from the minimization that indeed $\theta \simeq 0$ for the considered range of small to intermediate $V_{sp}/4t$. For

this reason, and to simplify the notation, we fix θ and α to zero.

With the LF transformation $U = \exp[-S_2(\gamma)]$ we obtain

$$\tilde{H} = E_0 + H_{\text{LF}} + H_{V_x} + H_{V_z} + H_{V_x V_z} \quad (19)$$

where $E_0 = -\frac{1}{2}NE_{2l} - NV_z n_b$, and

$$\begin{aligned} H_{\text{LF}} = & -t \sum_{\langle ij \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} e^{\frac{V_x}{E_{2l}^*} \gamma (b_i^\dagger - b_i)} e^{-\frac{V_x}{E_{2l}^*} \gamma (b_j^\dagger - b_j)} \\ & - V_{\text{eff}} \sum_i c_{i,\uparrow}^\dagger c_{i,\uparrow} c_{i,\downarrow}^\dagger c_{i,\downarrow} \\ & - \mu_{\text{LF}} \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} + E_{2l}^* \sum_i b_i^\dagger b_i \end{aligned} \quad (20)$$

with

$$H_{V_x} = (1 - \gamma) V_x \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} (b_i^\dagger + b_i) \quad (21)$$

$$H_{V_z} = V_z \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i,\sigma} - n/2) (b_i^\dagger b_i - n_b) \quad (22)$$

$$H_{V_x V_z} = -\gamma \frac{V_x V_z}{E_{2l}^*} \sum_{i,\sigma,\sigma'} (c_{i,\sigma}^\dagger c_{i,\sigma} - n/2) c_{i,\sigma'}^\dagger c_{i,\sigma'} (b_i^\dagger + b_i) \quad (23)$$

where the effective chemical potential is given by

$$\begin{aligned} \mu_{\text{LF}} = & \mu + V_z/2 + \gamma(2 - \gamma) \frac{V_x^2}{E_{2l}^*} \\ & - (1 - n) V_z \left(\gamma \frac{V_x}{E_{2l}^*} \right)^2 - V_z n_b \end{aligned} \quad (24)$$

The induced electronic interaction V_{eff} is now

$$V_{\text{eff}} = 2 \frac{V_x^2}{E_{2l}^*} \gamma \left[(2 - \gamma) - \gamma(3 - n) \frac{V_z}{E_{2l}^*} \right] - U, \quad (25)$$

where we note that the Hubbard term H_{e-e} has been unaffected by the above transformations of the electron-two level system coupling terms, due to the fact that it is simply a product of local densities. The local repulsion therefore merely diminishes the effective attraction by U .

If $\gamma = 1$, the first term within brackets in Eq. (25) coincides with the well-known result from the exact mapping of the Holstein model to the attractive Hubbard model in the high-frequency limit ($E_{2l} \rightarrow \infty$). The second term in the brackets $\propto V_z$ is always repulsive and suppresses T_c for increasing field. The electric field dependence enters through V_x , V_z , E_{2l}^* and the implicit dependence of γ on E_{sp} .

We have now achieved the desired result of expressing the Hamiltonian in terms of an effective BCS-like interaction between electrons, at the cost of introducing bosonic phase factors into the hopping matrix elements.

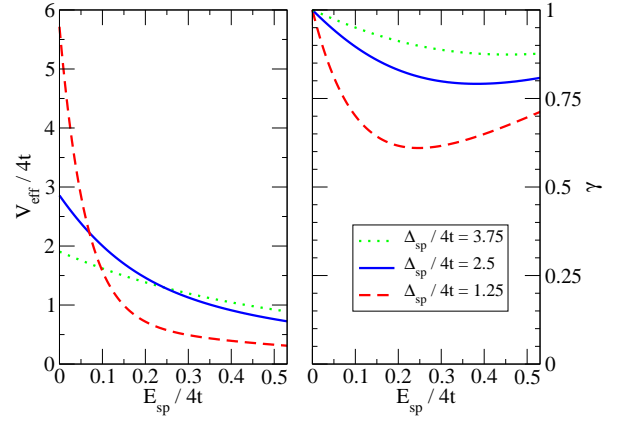


FIG. 2: Left panel: Effective pair interaction $V_{\text{eff}}/4t$ vs. normalized electric field energy $E_{sp}/4t$ for various excitation energies Δ_{sp} of the local two-level systems in layer $L1$. The dielectric constant $\epsilon = 100$ controls the increase of charge density in the metallic layer $L2$ with electric field (cf. Eqs. (38)–(39)), whereby we chose a bandwidth $4t = 400$ meV, a dipole length $d_{sp} = 2$ Å (for charge transfer excitations), and a lattice constant $a = 4$ Å. The coupling of the dipoles to the conduction electrons is fixed at $V_{sp}/4t = 1.89$ which corresponds to a spatial distance $r/a = 1.5$ (cf. Eq. (40)). Right panel: variational parameter γ vs. normalized electric field $E_{sp}/4t$, where γ is found from the minimization of the free energy (rhs of Eq. (26)).

We begin by setting $U = 0$ and investigate the magnitude of the attractive interaction obtainable by polarizing the two level systems. In Fig. 2 we illustrate how V_{eff} depends on applied electric field. The main point is physically obvious: if the electric field is sufficiently large, it polarizes the electric dipoles in $L1$ and suppresses the Little-type mechanism. We also note that if the bare excitation energy Δ_{sp} of the dipoles in the insulating layer is small, the intrinsic low-field pairing strength can be quite large, up to several electron volts. However Δ_{sp} should not be set to considerably smaller values than in Fig. 2 in order to guarantee the condition that the occupation of the excited state is negligible.

In the second step we introduce an exactly solvable test Hamiltonian H_{test} and determine the fields in H_{test} through a Bogoliubov inequality for the free energy F of the model system [25]:

$$F \leq F_{\text{test}} + \langle \tilde{H} - H_{\text{test}} \rangle_{\text{test}} \quad (26)$$

where $\langle \rangle_{\text{test}}$ signifies the thermodynamic average with the test Hamiltonian. We already anticipate the result of this variational scheme [26] and write

$$\begin{aligned} H_{\text{test}} = & E_{0,\text{test}} - t_{\text{eff}} \sum_{\langle ij \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} - \mu_{\text{LF}} \sum_i c_{i,\sigma}^\dagger c_{i,\sigma} \\ & + \left(\Delta \sum_i c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger + h.c. \right) - \Delta \sum_i \langle c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger \rangle \\ & + E_{2l}^* \sum_i b_i^\dagger b_i \end{aligned} \quad (27)$$

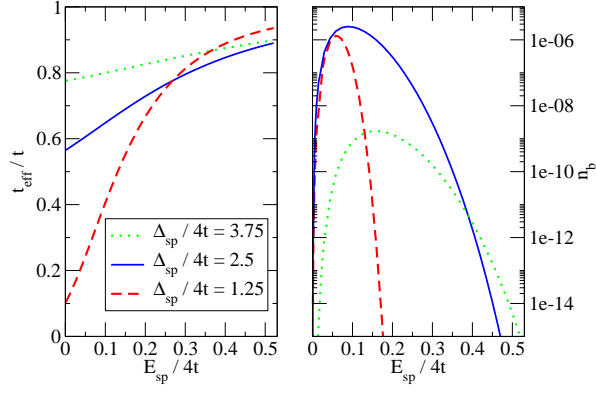


FIG. 3: Left panel: Effective hopping t_{eff}/t vs. normalized electric field energy $E_{\text{sp}}/4t$ at the transition temperature T_c ; all parameters are identical to those of Fig. 2. Right panel: bosonic occupation number n_b (the relative number of inverted two-level systems per site) vs. normalized electric field energy $E_{\text{sp}}/4t$ at the transition temperature T_c .

with

$$E_{0,\text{test}} = E_0 - \frac{N}{4} n^2 V_{\text{eff}} \quad (28)$$

$$t_{\text{eff}} = t \exp \left[- \left(\frac{V_x}{E_{2l}^*} \gamma \right)^2 \coth \left(\frac{\beta E_{2l}^*}{2} \right) \right] \quad (29)$$

We have assumed s -wave pairing for simplicity. The associated gap equation then reads

$$\Delta = V_{\text{eff}} \sum_{\mathbf{k}} \frac{\Delta}{2E_{\mathbf{k}}} \tanh \frac{E_{\mathbf{k}}}{2T} \quad (30)$$

and the Bogoliubov quasiparticle dispersion

$$\begin{aligned} E_{\mathbf{k}} &= \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2} \\ \xi_{\mathbf{k}} &= \varepsilon_{\mathbf{k}} - \mu_{\text{LF}} \\ \varepsilon_{\mathbf{k}} &= -2 t_{\text{eff}} (\cos k_x + \cos k_y) \end{aligned} \quad (31)$$

To understand qualitatively the physics of the correlations induced by interaction of the metallic layer with the 2-level systems in $L1$, we display in the left panel of Fig. 3 the magnitude of the renormalized hopping t_{eff} . The band narrowing can be rather significant for small excitation energies Δ_{sp} but for the parameters of greatest interest will turn out to be only a factor of 1–5.

The fields still depend on the parameter γ ; correspondingly the rhs of relation Eq. (26) has to be minimized with respect to γ . For this purpose we need the explicit form of F_{test} :

$$F_{\text{test}} = E_{0,\text{test}} + \frac{1}{\beta} N \ln \left(1 - e^{-\beta E_{2l}^*} \right) + F_{\text{BCS}} \quad (32)$$

with

$$\begin{aligned} F_{\text{BCS}} &= - \frac{2}{\beta} \sum_{\mathbf{k}} \ln (1 + e^{-\beta E_{\mathbf{k}}}) \\ &\quad - \sum_{\mathbf{k}} \left(E_{\mathbf{k}} - \xi_{\mathbf{k}} + \Delta \langle c_{-k,\downarrow} c_{k,\uparrow} \rangle \right) \end{aligned} \quad (33)$$

Since we have chosen $E_{0,\text{test}}$ so as to guarantee the relation $\langle \hat{H} - H_{\text{test}} \rangle_{\text{test}} = 0$, the variation reduces to finding the optimal value of γ from the minimization of F_{test} :

$$\gamma = \frac{n(n+2)}{n(n+2) + n(n+1)(2-n)(V_z/E_{2l}^*) + \delta(\gamma)} \quad (34)$$

where

$$\delta(\gamma) = 2 \frac{\bar{\varepsilon}}{E_{2l}^*} \coth \left(\frac{\beta E_{2l}^*}{2} \right) \quad (35)$$

and

$$\bar{\varepsilon} = \sum_k \frac{\varepsilon_k}{1 + e^{\beta \xi_k}} \quad (36)$$

For the range of parameters considered in our evaluation the function $\delta(\gamma)$ can be neglected with respect to the other terms in the denominator of Eq. (34). This allows us to calculate γ algebraically from Eq. (34). The validity of this approximation has been proved by iterating the implicit Eq. (34). Fig. 2 (right panel) displays the decrease of γ with increasing E_{sp} for various values of Δ_{sp} at fixed $V_{\text{sp}}/4t = 1.89$.

Finally the assumption below Eq. (11) that the bosonic occupation number $n_b = \langle b_i^\dagger b_i \rangle$ is very small is in fact justified a posteriori for temperatures up to the transition temperature T_c . In the considered parameter range of the two-level splitting Δ_{sp} and of the applied gate field E_{sp} , n_b is always smaller than 10^{-5} . Typical field dependences of n_b are displayed in the right panel of Fig. 3.

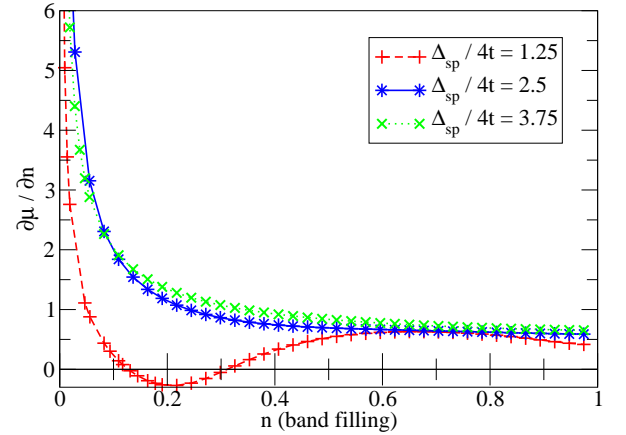


FIG. 4: The derivative of the chemical potential with respect to particle density, $\partial\mu/\partial n$, versus particle density n at the respective T_c , calculated in Sec. II. All parameters are identical to those of Fig. 2. For a positive derivative, the normal and superconducting states are globally stable in the vicinity of the transition.

The effective model does not implement the long-range part of the Coulomb interaction. A model with purely local interactions, however, has a tendency towards phase

separation. In order to investigate if the transition from the normal to the superconducting state is a transition between global minima of the free energy, we evaluated the derivative of the chemical potential with respect to carrier density. In this work, we focus on the transition into the superconducting state and not on the evolution of the superconducting state at lower temperatures. Then it is sufficient to discuss the stability in the vicinity of T_c . Fig. 4 illustrates our conclusion that the derivative of the chemical potential with respect to particle density is always positive for $\Delta_{sp}/4t$ larger than approximately 1.4. Correspondingly, the transition into the superconducting state is not preempted by a competing transition into a phase separated state. At somewhat lower values of $\Delta_{sp}/4t$, the phase separation will probably be suppressed by the non-local part of the Coulomb interaction. As discussed in the following section, the relevant values of $\Delta_{sp}/4t$ for a sufficiently strong interface-mediated pairing appear in the regime where $\partial\mu/\partial n$ is positive.

II. RESULTS

In order to present the numerical results in the physically relevant range of control parameters, we have to relate microscopic quantities to laboratory parameters, such as the dielectric constant ϵ of the insulating layer, the dipole length d_{sp} of the two-level systems, and the distance r from the two-level systems to the sites of the conducting layer. Furthermore we have to establish a relation between the electric field energy E_{sp} (see Eq. (1)) and the number of charge carriers in $L2$. In our calculation we assume that the charge carrier density is a linear function of the electric field with a field independent capacitance C of the dielectric $L1$: $Q = CV$, where V is the voltage drop across the dielectric and Q is the total, accumulated charge at the interface in $L2$. Then, the charge per square unit cell is

$$n = C \frac{\mathcal{E}d}{e} \frac{a^2}{A} \quad (37)$$

where a is the lattice constant, A is the area of $L2$ and d its thickness (cf. Fig. 1). With $C = \epsilon_o \epsilon A/d$ and Eq. (1) we establish

$$n = c \frac{E_{sp}}{4t} \quad (38)$$

with

$$c = \epsilon_o \epsilon \frac{a^2}{e^2} \frac{4t}{d_{sp}} \quad (39)$$

The interaction energy between the dipoles next to the interface and the electric field of a charge carrier on the nearest site is

$$V_{sp} = \frac{1}{4\pi\epsilon_0} \frac{e^2 d_{sp}}{r^2}. \quad (40)$$

We note that dynamical screening of the interaction V_{sp} should be included in order to get more precise estimates. Although this will reduce somewhat the high values of T_c in our evaluation, it will not alter the qualitative behavior of the T_c -dependence on the gate field (see below).

Finally, the excitation energy of the dipoles has to be identified. A generic dielectric is not composed of a single species of well-defined 2-level systems. Dipole excitations at various energies are always present. We now address excitations in three different energy ranges: for 10 eV (low atomic excitations with dipole length $d_{sp} \simeq 1$ Å), in the 1 eV range (charge transfer excitations with $d_{sp} \simeq 2$ Å), and in the meV range (ionic displacement in atomic clusters with $d_{sp} \simeq 0.1$ Å).

A. Ionic displacement

In dielectrics a displacement of ions, well localized at atomic positions, usually accounts for the high dielectric constant. Such displacements in atomic clusters typically correspond to a dipole length of the order of $d_{sp} \simeq 0.1$ Å and a small excitation energy. In this case, the excitation energy is related to ϵ and d_{sp} through $\Delta_{sp} = 8\pi e^2 d_{sp}^2 / (a^3 (\epsilon - 1))$. This relation follows directly from the polarization density $\langle P \rangle$ of the dielectric (with a cubic unit cell of volume a^3) in linear response: $\langle P \rangle = e d_{sp} \langle s_i^\dagger p_i + p_i^\dagger s_i \rangle / a^3 = (2 e^2 d_{sp}^2 / a^3 \Delta_{sp}) \mathcal{E}$ where $\langle P \rangle = (\epsilon - 1) / 4\pi \mathcal{E}$ holds. Ionic displacements may have energies of the order of 10 meV (for ϵ of the order of 20). However, the induced pair interaction is far too small (see Fig. 5) to find sizable transition temperatures. It is the repulsive term in $V_{eff}/4t$ of Eq. (25) which very effectively impedes a transition to the superconducting state for such small values of Δ_{sp} .

B. Charge transfer excitations

In order to realize a sizable T_c of the order of 100 K, excitations at intermediate energy and sufficiently large dipole length have to be available for polarization. Charge transfer excitations in the dielectrics are found at these energies — e.g. for the transition metal (TM) oxides at energies of the order of 1 eV, the charge transfer gap. Although these excitations of, for example, a TM-oxygen plaquette or octahedron become delocalized through hybridization, we assume that most states near the interface have been localized by disorder and local strain [27]. Furthermore localized bound states below the charge transfer gap are conceivable. It is not the focus of our present investigation to identify these local excitations for a specific material. We rather point out that such processes are possible and then evaluate T_c as a function of their respective energy.

We intend to focus on this latter type of localized charge transfer excitations. For the evaluation we now

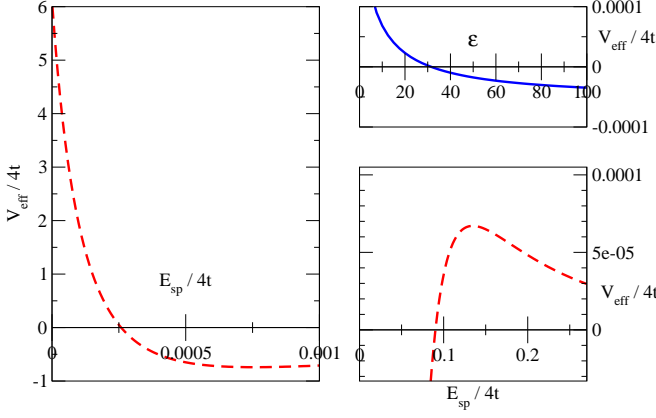


FIG. 5: Ionic displacement in atomic clusters: induced pairing interaction $V_{\text{eff}}/4t$ versus electric field energy $E_{\text{sp}}/4t$ for $\epsilon = 10$, $d_{\text{sp}} = 0.1 \text{ \AA}$ and $r/a = 1$ (which corresponds to $V_{\text{sp}}/4t = 0.2125$). Left and lower right panels show different scales. Upper right panel: Pairing interaction versus dielectric constant ϵ for charge density $n = 0.5$.

fix the following parameters: the bandwidth, the dipole length, and the lattice constant:

$$\begin{aligned} 4t &= 400 \text{ meV} \\ d_{\text{sp}} &= 2 \text{ \AA} \\ a &= 4 \text{ \AA} \end{aligned} \quad (41)$$

Here, we chose a bandwidth and lattice constant typical of the high- T_c cuprates and many other oxides, and we take a dipole length which corresponds to the inter-atomic oxygen-TM distance. For excitation energies Δ_{sp} of more than 0.2 eV, the primary polarization processes are electronic in nature.

In Fig. 6 the transition temperature to the superconducting state is displayed as a function of the excitation energy. In the range of small, increasing values of Δ_{sp} we observe a strong enhancement of T_c whereas the transition temperature decreases with excitation energies $\Delta_{\text{sp}}/4t$ above ≈ 2.5 . The latter observation is expected since the pairing interaction V_{eff} is inversely proportional to the excitation energy for large Δ_{sp} . For small Δ_{sp} , the repulsive term (second term in V_{eff} , cf. Eq. (25)) dominates and suppresses the transition to the superconducting state for a finite value of Δ_{sp} . Note that the finite longitudinal pseudospin-charge V_z is decisive for the decay of T_c at small excitation energies, outside the regime where the Holstein model is appropriate.

For small increasing electric field, the transition temperature is raised due to the accumulation of charge in the metallic layer (cf. Fig. 7). The electric field strength is directly related to the band filling or induced areal charge density. Strong electric fields with sizable band filling lower the transition temperature as the repulsive term in V_{eff} is enhanced and, moreover, the effective level splitting is enlarged. In fact, as seen from the $\Delta_{\text{sp}}/4t = 1.25$ curve in Fig. 7 there are two scales for the suppression of

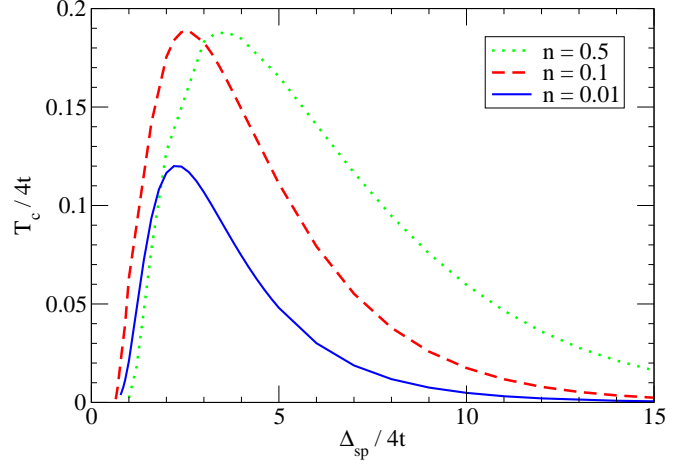


FIG. 6: Charge transfer excitations: transition temperature $T_c/4t$ versus excitation energy $\Delta_{\text{sp}}/4t$. The three curves present T_c for small and intermediate band filling. The dielectric constant is $\epsilon = 100$, which implies $c = 1.87$ for the considered set of parameters (see Eq. (41)). The coupling of the dipoles to the conduction electrons is fixed to $V_{\text{sp}}/4t = 1.89$ which corresponds to a spatial distance $r/a = 1.5$ (cf. Eq. (40)).

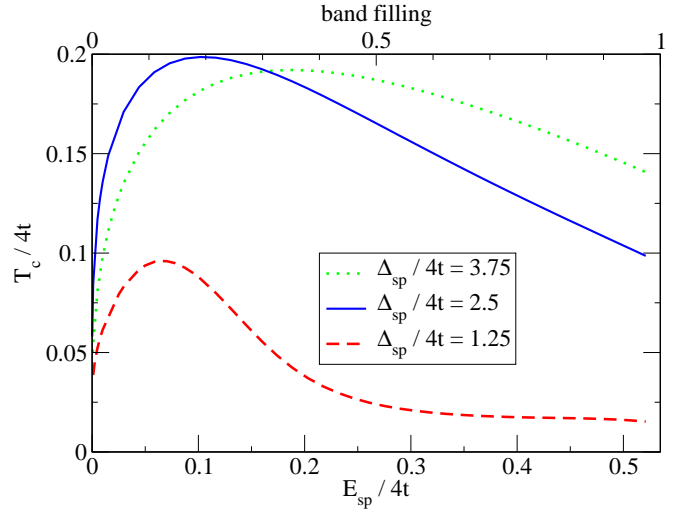


FIG. 7: Charge transfer excitations: transition temperature $T_c/4t$ versus electric field energy $E_{\text{sp}}/4t$ and band filling n , lower axis and upper axis, respectively. The three curves present different dielectrics which are characterized by different excitation energies only, other parameters are fixed for comparison. The dielectric constant ϵ is 100 and $V_{\text{sp}}/4t = 1.89$ ($r/a = 1.5$).

T_c at higher fields. The lower scale is set by the repulsive term in V_{eff} and is also responsible for the observed decay of T_c in the two further curves (with $\Delta_{\text{sp}}/4t = 2.5$ and 3.75). In this regime, T_c is being suppressed primarily by the increasing repulsion V_z between the polarized dipoles and the 2D electrons, which scales with the applied field.

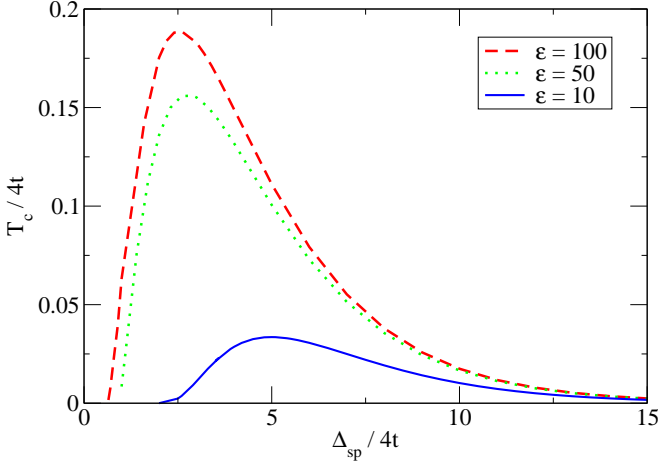


FIG. 8: Charge transfer excitations: transition temperature $T_c/4t$ versus excitation energy $\Delta_{sp}/4t$. The three curves present different dielectrics ($\epsilon = 10, 50, 100$). The band filling is fixed at $n = 0.1$, and the interaction $V_{sp}/4t = 1.89$ corresponds to $r/a = 1.5$.

The larger scale, which is responsible for the slow decay at even higher fields, is set by $\Delta_{sp}/4t$, and corresponds to the eventual saturation of the dipole moment of the 2-level systems.

The nonmonotonic dependence on filling or electric field is reflected in the varying height of the three different curves in Fig. 6. However more striking is the small variation of the position of the maxima in Fig. 6 with filling (from 0.01 to 0.5). A value of $\Delta_{sp} \simeq 1$ eV seems to be optimal for a bandwidth of $4t = 400$ meV. This optimal excitation energy in units of the band width is approximately

$$\Delta_{sp}^{\text{opt}}/4t \simeq 2.5 \quad (42)$$

Δ_{sp}^{opt} is weakly dependent on the parameters V_{sp} , d_{sp} and ϵ which mostly influence the maximum value of T_c . For fixed charge density, dielectrics with larger ϵ display a higher transition temperature (for given Δ_{sp}), see Fig. 8, as the electric field necessary to create the charge density is smaller, accounting for a larger V_{eff} .

An increasing dipole charge-carrier interaction V_{sp} is not only responsible for an enhancement of T_c but, for sufficiently large V_{sp} , also for a “retarded” initial increase of T_c with electric field (see Fig. 9). Again, this observation may be traced back to the field and interaction dependence of the repulsive term in V_{eff} .

For direct comparison with experimental devices, we note that the gate voltage is related to the electric field energy plotted in the figures through $E_{sp}/4t = ed_{sp}V/d$ where d is the thickness of the dielectric gate. As a concrete example for a dielectric gate layer, we take SrTiO_3 . Breakdown fields of 4×10^7 V/m are reported for this material with a low- T dielectric function of order 100 [28]. The maximum of the T_c versus electric field energy curves

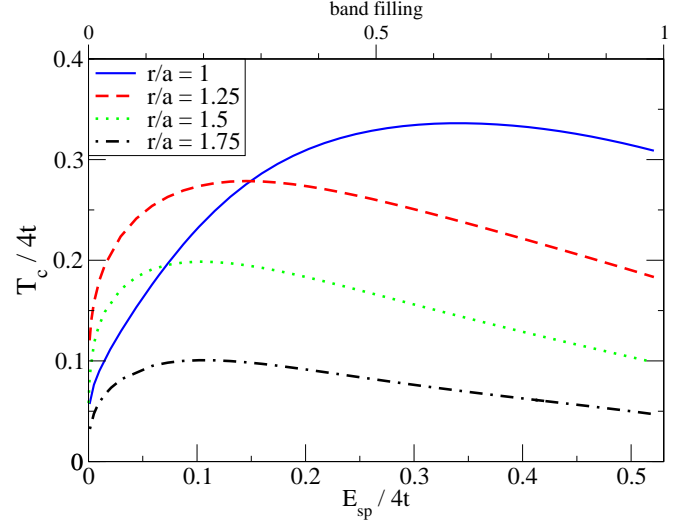


FIG. 9: Charge transfer excitations ($d_{sp} = 2$ Å, $\Delta_{sp}/4t = 2.5$, $\epsilon = 100$): transition temperature $T_c/4t$ versus electric field energy $E_{sp}/4t$, parameterized by r/a . The corresponding V_{sp} is in the intermediate coupling range: $V_{sp}/4t = 4.25$ (corresponds to $r/a = 1$), $V_{sp}/4t = 2.72$ ($r/a = 1.25$), $V_{sp}/4t = 1.89$ ($r/a = 1.5$), $V_{sp}/4t = 1.39$ ($r/a = 1.75$).

occurs for $n = 0.2$ at about 2×10^8 V/m. Thus the required fields for the *maximum* T_c are only about 5 times higher than those already realized in this system. Given that breakdown occurs due to “pinhole”-type defects in the films, it seems to us that the manufacture of samples with the required breakdown fields is challenging but far from impossible.

We conclude this subsection with a brief discussion of the consequences that a nonzero local interaction U within the charge-carrier layer $L2$ has on the reduction of T_c in a weak-coupling evaluation. As shown in Eq. (25), such a repulsive Hubbard-type interaction does not modify the field dependence of the effective interaction V_{eff} , but just adds a constant $-U$. For weak interaction $U/4t \lesssim 1$, the effective attraction V_{eff} is reduced but not fully suppressed for small to intermediate fields (cf. Fig. 2) and corresponding filling. This observation is reflected in the field and filling dependence of T_c (see Fig. 10): T_c is reduced for small to intermediate fields and suppressed for strong field-induced doping. As a consequence of the field-dependent reduction of T_c , the maxima are shifted towards lower values of filling, from about $n = 0.2$ at $U = 0$ to $n = 0.1$ at $U/4t = 1$. The required fields for the *maximum* T_c are reduced similarly.

C. Atomic excitations

At high energies, we encounter atomic excitations, such as the $2p$ to $3s$ transition of O^{2-} states in the metal oxides. These states are treated in exactly the same way in the current theory, but are characterized by small dipole

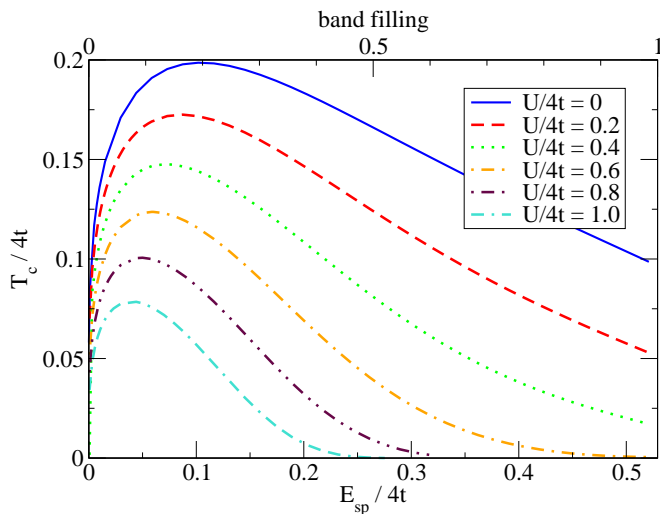


FIG. 10: Charge transfer excitations: transition temperature $T_c/4t$ versus electric field energy $E_{sp}/4t$ and band filling n , lower axis and upper axis, respectively. A local electronic interaction U (within layer $L2$) is included in a weak coupling evaluation. The dielectric constant ϵ is 100 and $V_{sp}/4t = 1.89$ ($r/a = 1.5$).

lengths $d_{sp} \sim 1 \text{ \AA}$ and large 2-level splittings $\Delta_{sp} \sim 10 \text{ eV}$. Polarizing such dipoles is difficult and T_c 's are correspondingly small. Comparison of Fig. 11 for parameters consistent with atomic polarizations with Fig. 9 for charge transfer excitations makes the distinction of the two scenarios evident. In the atomic case, T_c is so small that an observable effect may be found only for the smallest value of r/a . Moreover, the excitation energy is so high that a decrease of T_c is not seen, even for the largest electric fields. Of course, when band filling is above half filling, the transition temperature will decrease with increasing field. However these field strengths are beyond electrical breakdown.

III. CONCLUSIONS

We have proposed that the field-induced 2DEG in a field effect device may become superconducting entirely due to pair interactions with a proximate insulating layer with high polarizability. In the general case, properties of a DS-channel embedded in an oxide field effect transistor will then be controlled not only by the electronic and structural properties of the DS-channel, as is usually assumed, but can furthermore be strongly influenced by the gate insulator or by other adjacent dielectric layers. The choice of the gate dielectric layer may then influence the device behavior of a field effect transistor far beyond controlling the maximum gate polarization and gate current.

For a concrete model of electrons in a 2D layer interacting with 2-level systems at the interface with the

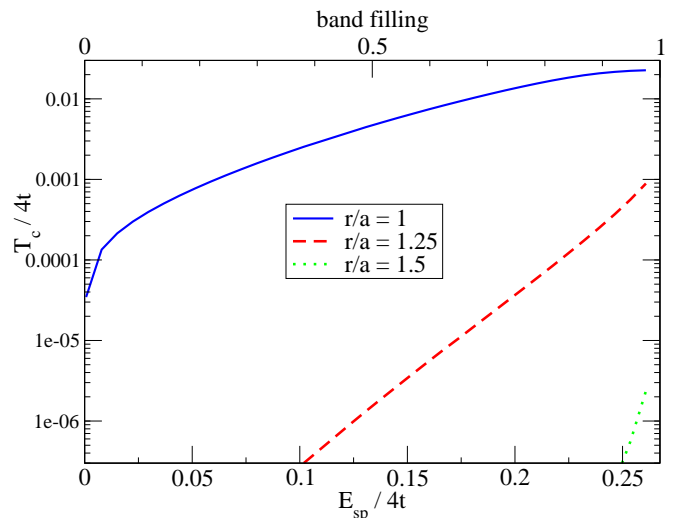


FIG. 11: Atomic excitations ($d_{sp} = 1 \text{ \AA}$, $\Delta_{sp} = 10 \text{ eV}$, $\epsilon = 100$): transition temperature $T_c/4t$ versus electric field energy $E_{sp}/4t$, parameterized by r/a : $V_{sp}/4t = 2.125$ (corresponds to $r/a = 1$), $V_{sp}/4t = 1.36$ ($r/a = 1.25$), $V_{sp}/4t = 0.94$ ($r/a = 1.5$).

insulator, we calculated the superconducting critical temperature, which displays as a function of applied field a steep initial rise and subsequent decay. The rise is caused by the increasing density of charge carriers swept to the interface by the electric field and the decay is due to the interaction of the field-induced dipoles with the charge carriers. The optimal values of the field or gate voltage, as well as sample dimensions and dielectric properties, were discussed in some detail within the framework of this model.

The goal of these model calculations was to establish the plausibility of superconductivity in field-effect devices enhanced or induced by the presence of a polarizable interface, and to investigate the magnitude of the critical temperature and likely dependence on external field and materials properties. We recognize, however, that several potentially important aspects of the physics are not present in the model used. These include long-range Coulomb interactions, dynamics of the dielectric screening, and correlations in the 2DEG. We anticipate that the effects of long-range Coulomb interactions are less important in the present case than in 3D metallic superconductors due to the larger dielectric constants in the insulating material, but this must clearly be justified by a legitimate calculation of the true Coulomb pseudopotential entering the MacMillan formula. Screening of the bare electron-dipole interaction V_{sp} must also be included; we expect, however, that the form of the dependence of T_c on the electric field will not change significantly (see Fig. 9). The inclusion of a repulsive local interaction U does not qualitatively change this form either. However it reduces T_c (by a factor of 2 for $U/4t = 0.8$) and it shifts the optimal value of the field-induced doping to lower levels (cf.

Fig. 10).

If the effective on-site Coulomb repulsion in the drain-source layer is much larger than we have considered, s -wave superconductivity will be completely suppressed. It is still tempting, however, to regard the starting Hamiltonian (3)–(7) as the hopping of correlated electrons (as in the $t - J$ model) where Coulomb interactions have already been accounted for. In this case, however, one must implicitly assume that doubly occupied sites have been projected out, so that non-retarded s -wave superconductivity is impossible. Modelling superconductivity within this framework in higher-angular momentum pair channels will require including interactions among the two-level systems at the interface, so as to produce a nonlocal pair potential. While we have not calculated these effects explicitly, as they are technically significantly more difficult, our expectation is that the creation and eventual suppression of the paired state by the electric field will be qualitatively similar to what we have calculated. This expectation is supported by the observation that an increase in T_c with doping has to result trivially from an enhanced carrier density. Moreover, the buildup of a field-dependent repulsive interaction V_z has to take place due to the eventual saturation of the dipole moments with electric field, even when the two-level systems interact. Investigations along these lines are in progress.

In addition, our considerations can in principle be applied to other, more weakly correlated systems than the copper oxides. Our model may be used to treat situations in which the DS-channel contains an attractive s -wave in-

teraction besides the interface-mediated pairing. In this case we expect a qualitatively similar behavior with a nonmonotonic T_c .

According to our calculations, devices with thickness of the insulating layer of order 1000 Å subjected to voltages of order ~ 20 V could display superconductivity, if an optimal material can be found with a sufficiently large low frequency dielectric constant of order 30-100 and strong quasilocalized electronic modes of energy $\Delta_{sp}/4t \sim 2.5$ [29]. With a 20 V gate field and a typical 18 nF capacitance of a 0.03 cm² gate dielectric (1000 Å), this would correspond to a surface charge density of roughly 12 $\mu\text{C}/\text{cm}^2$. It is now routine to fabricate epitaxial high ϵ oxide dielectrics, such as SrTiO₃ with polarizations in the range of 10-40 $\mu\text{C}/\text{cm}^2$ [8]. Interface-mediated 2D superconductivity therefore seems to us to be plausibly within reach if good interfaces can be manufactured.

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